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Title: Enhanced Multiple Exciton Generation in PbS CdS Janus-like Heterostructured Nanocrystals

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Enhanced Multiple Exciton Generation in PbS|CdS Janus-like Heterostructured Nanocrystals

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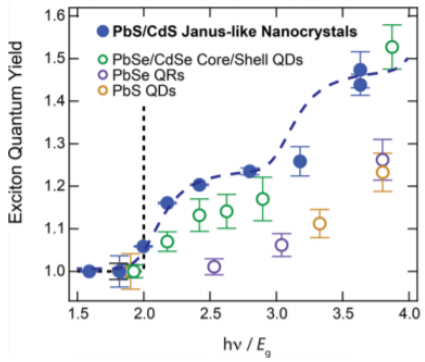
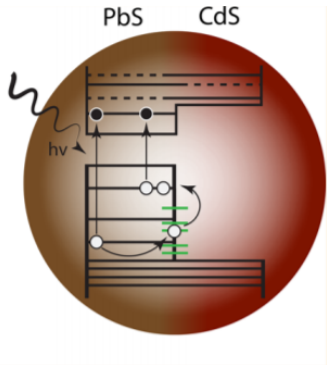
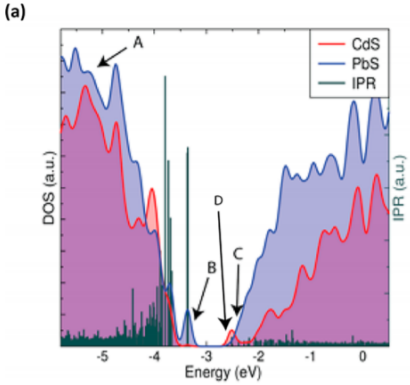
IC Annual Report for w18_solarcells

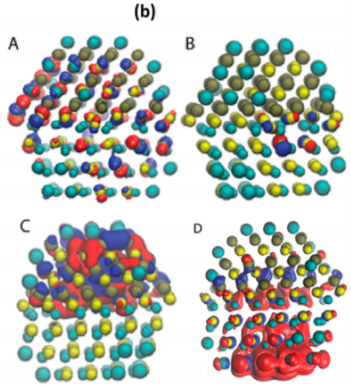
1. **Conducted state-of-the-art *ab initio* calculations on PbS|CdS Janus nanoparticles, illustrating enhanced Multiple Exciton Generation leading to high solar cell efficiencies**

2. **Demonstrated the importance of effective Coulomb interactions and a reduced hot exciton cooling rate, through analysis of the valence band interfacial states**









D.M. Kroupa, G.F. Pach, Márton Vörös, Federico Giberti et al, ACS Nano 12, 10084-10094 (2018)

We used first principles simulations to guide engineering of nanoparticle solar cells by investigating MEG in NP heterostructures